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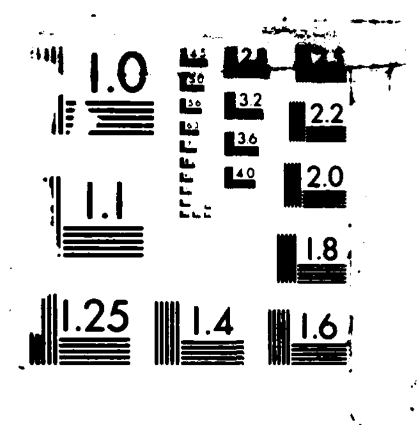
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by

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H. R. Lerche and D. Siegmund
University of Freiburg and Stanford University

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DEPARTMENT OF STATISTICS
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Approximate Exit Probabilities for a Brownian Bridge on a Short Time Interval, and Applications

by

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To Henry Daniels on his 75th Birthday

Summary.

Let T be the first exit time of Brownian motion $W(t)$ from a region $\mathcal{R}$ in d-dimensional Euclidean space having a smooth boundary. Given points ξ_0 and ξ_1 in $\mathcal{R}$, ordinary and large deviation approximations are given for $\Pr\{T < \varepsilon | W(0) = \xi_0, W(\varepsilon) = \xi_1\}$ as $\varepsilon \to 0$. Applications are given to hearing the shape of a drum, approximating the second virial coefficient, and Monte Carlo estimation of first passage distributions for Brownian motion.

Key Words and Phrases: Brownian bridge, first passage, hearing the shape of a drum, Monte Carlo methods.

1. Introduction.

Let $W(t), 0 \le t < \infty$, denote Brownian motion in $\mathbb{R}^d$ with $W(0) = \xi_0$. For $t > 0$ and events A in the σ-algebra generated by $W(s), 0 \le s \le t$, let

$$P^{(t)}_{\xi_0,\xi_1}(A) = \Pr(A|W(0) = \xi_0, W(t) = \xi_1).$$

Assume that ξ_0 and ξ_1 belong to some region $\mathcal{R}$ with a smooth boundary $\partial\mathcal{R}$, and let T denote the time W first leaves $\mathcal{R}$, i.e., $T = \inf\{t : W(t)\epsilon\partial\mathcal{R}\}$. The principal subject of this paper is the asymptotic behavior of

$$P^{(t)}_{\xi_0,\xi_1}\{T < t\} \tag{1.1}$$

as $t \to 0$ and the ξ_i are at a distance $O(t^{1/2})$ from each other and from $\partial\mathcal{R}$. A secondary consideration is the case where the distances of the ξ_i to the boundary and each other are fixed as $t \to 0$.

This problem for $d = 2$ and $\xi_0 = \xi_1$ arises naturally in the beautiful paper of Kac (1966), who was concerned with the behavior for small t of

$$\Sigma \exp(-\lambda_k t), \tag{1.2}$$

where the λ_k are eigenvalues of the Laplacian acting on functions having domain $\mathcal{R}$ and vanishing on $\partial\mathcal{R}$. Kac shows that as $t \to 0$ (1.2) has an expansion of the form $c_1 t^{-1} + c_2 t^{-1/2} + o(t^{-1/2})$, where c_1 and c_2 are numerical multiples of $|\mathcal{R}|$, the area of $\mathcal{R}$, and $|\partial\mathcal{R}|$, the length of $\partial\mathcal{R}$, respectively. He argues heuristically that the next term is $(1-h)/6$, where h is the number of holes in $\mathcal{R}$. For more detailed results along these lines, see Louchard (1968), McKean and Singer (1967), Stewartson and Waechter (1971), and Smith (1981). Of these, only Louchard attempts a probabilistic analysis, and his argument appears to contain a mistake.

Starting from the physical problem of evaluating the second virial coefficient of a hard sphere gas, Handelsman and Keller (1966) arrive at essentially Kac's mathematical problem, for the case $d = 3, \xi_0 = \xi_1$, and $\mathcal{R}$ the region exterior to a sphere. They derive what in Kac's problem corresponds to c_3 and the next term, $c_4 t^{1/2}$. Although their method

does not seem capable of being turned into a rigorous proof, minor modifications appear to produce correct answers under much more general conditions.

A problem having a rather different flavor is to estimate (1.1) by a Monte Carlo experiment, when t is not necessarily small and the ξ_j are not necessarily close to the boundary of $\mathcal{R}$. A natural approach is to partition the time interval $[0, t]$ at $m + 1$ equally spaced points $t_i = it/m$, $i = 0, \ldots, m$ and count the relative frequency with which a simulated path $W(t_i), i = 0, 1, \ldots, m$, leaves $\mathcal{R}$. The bias introduced by discretization is typically $O(m^{-1/2})$ (cf. Siegmund, 1985, Chapter X, or Hogan, 1984); and increasing m sufficiently to reduce this bias to an acceptable level is computationally time consuming. However, having observed $W(t_{i-1}) = \xi_{i-1} \epsilon \mathcal{R}$ and $W(t_i) = \xi_i \epsilon \mathcal{R}$, one can use an approximation to (1.1) and a single uniform random variable to simulate the event that $W(s)$ leaves $\mathcal{R}$ for some s in the time interval (t_{i-1}, t_i). Although the original interval $[0, t]$ need not be short, the various subintervals $[t_{i-1}, t_i]$ are, provided m is large.

Note that this technique does not require that W be exactly Brownian, but only that it be approximately so over short time intervals. The basic idea is in principle applicable to diffusion processes and to certain Gaussian processes which are locally Brownian.

As noted by Kac, in the case $\xi_0 = \xi_1$, the probability (1.1) is to a first order approximation equal to the probability that $W(s)$ for some $0 \le s \le t$ touches the plane tangent to $\mathcal{R}$ at the point of $\partial\mathcal{R}$ closest to ξ_0. Section 2 contains the first term of an Edgeworth type expansion for this probability when ξ_0 and ξ_1 are not necessarily the same. A large deviation approximation is also given. Section 3 gives the substantially more complicated second Edgeworth term. For computational simplicity only the case $\xi_0 = \xi_1$ is considered there, but this case illustrates the method and contributes to the Kac and Handelsman–Keller problems. The method used in Sections 2 and 3 is a modification of that introduced by Siegmund and Yuh (1982) in a simple linear case and explored more thoroughly by Siegmund (1985).

Section 4 describes some illustrative Monte Carlo experiments. It can be read independently of Sections 2 and 3, except for an occasional reference to some of the basic notation and to the statements of Theorems 1 and 2.

2. Approximations to $P^{(t)}_{\xi_0,\xi_1}\{T < t\}$.

For ease of exposition we consider in detail only the case $d = 2$ and indicate in some remarks how the results are modified for general d.

Given $\xi_0, \xi_1 \epsilon \mathcal{R}$, close to $\partial\mathcal{R}$ and to each other, assume there exists a unique point on $\partial\mathcal{R}$ the sum of whose distances to the given points is a minimum. Consider the Cartesian coordinate system which has this point as its origin, the x– axis as tangent and the y–axis as outward normal to $\mathcal{R}$. There exists a function $y = f(x)$ such that locally near $(0,0)$ $\partial\mathcal{R}$ is given by the graph $(x, f(x))$. Let ξ_i have coordinates (x_i, y_i) in this coordinate system, and assume that $y_i < 0 (i = 0,1)$. It is easily seen that ξ_0 and ξ_1 satisfy $-x_0/|y_0| = x_1/|y_1|$. (A ray of light emanating from ξ_0 and reflecting off the x–axis at the origin passes through ξ_1.) Let $W(t)$ denote Brownian motion starting from $W(0) = \xi_0$, and define

$$T = \inf\{t : W_2(t) \geq f(W_1(t))\}. \tag{2.1}$$

In general, T is not the exit time of W from $\mathcal{R}$, but for ξ_0 close to $(0,0)$ it is with probability close to one. (A more precise estimate is given below.)

In order to study $P^{(\epsilon)}_{\xi_0,\xi_1}\{T < \epsilon\}$ it is convenient to use Brownian scaling to replace the given problem on the time interval $[0, \epsilon]$ by an equivalent one on $[0,1]$. Since $W(\epsilon t)/\epsilon^{1/2}$ is Brownian motion starting from $\tilde{\xi}_0 = \xi_0/\epsilon^{1/2}$, it is easy to see that

$$P^{(\epsilon)}_{\xi_0,\xi_1}\{T < \epsilon\} = P^{(1)}_{\tilde{\xi}_0,\tilde{\xi}_1}\{\tilde{T} < 1\}, \tag{2.2}$$

where $\tilde{\xi}_i = \xi_i/\epsilon^{1/2}$ $(i = 0,1)$ and

$$\tilde{T} = \tilde{T}_\epsilon = \inf\{t : W_2(t) \geq \epsilon^{-1/2} f(\epsilon^{1/2} W_1(t))\}. \tag{2.3}$$

To give a precise statement of our first result it is convenient to change our viewpoint slightly and regard f as given and the points ξ_i as variable.

Theorem 1. Assume f is twice continuously differentiable, $f(0) = f'(0) = 0$, and $f''(0) \neq 0$. Suppose $\xi_i = (x_i, y_i)$ $(i = 0,1)$ satisfy $y_i < 0$ $(i = 0,1)$ and $-x_0/|y_0| = x_1/|y_1|$, and converge to $(0,0)$ as $\epsilon \to 0$ in such a way that $\tilde{\xi}_i = \xi_i/\epsilon^{1/2}$ are fixed $(i = 0,1)$. Then for T defined by (2.1)

$$(2.4)\qquad P^{(\varepsilon)}_{\xi_0,\xi_1}\{T<\varepsilon\}=\exp(-2y_0y_1/\varepsilon)\Bigg\{1-f''(0)\Bigg[\varepsilon^{-1/2}|y_0y_1| \times\frac{\Phi[(y_0+y_1)/\varepsilon^{1/2}]}{\varphi[(y_0+y_1)/\varepsilon^{1/2}]}(1-\varepsilon^{-1}(x_1-x_0)^2)+\varepsilon^{-1}(x_0^2|y_1|+x_1^2|y_0|)+o(\varepsilon^{1/2})\Bigg]\Bigg\},$$

where Φ and φ are the standard normal distribution and density function respectively.

Proof. By virtue of (2.2) it suffices to consider the standardized problem on the time interval $[0,1]$, with fixed initial and terminal points $\tilde{\xi}_0=(\tilde{x}_0,\tilde{y}_0)$ and $\tilde{\xi}_1=(\tilde{x}_1,\tilde{y}_1)$, and $\tilde{T}$ defined by (2.3). To simplify the notation we consider only this standardized problem and omit the tildes for the rest of the proof. In this new notation, where all variables have tildes, but the tildes are omitted, (2.4) becomes

$$(2.5)\quad P^{(1)}_{\xi_0,\xi_1}\{T_\varepsilon<1\}=\exp(-2y_0y_1)\Bigg\{1-\varepsilon^{1/2}f''(0)\Bigg[|y_0y_1| \times\frac{\Phi(y_0+y_1)}{\varphi(y_0+y_1)}(1-(x_1-x_0)^2)+(x_0^2|y_1|+x_1^2|y_0|)+o(1)\Bigg]\Bigg\},$$

with T_ε defined by (2.3).

We begin with an informal calculation and provide a justification later. The argument proceeds from a suitable likelihood ratio identity. Let $\xi_1'=(x_1,|y_1|)$. The likelihood ratio of $W(s), s\le t$, under $P^{(1)}_{\xi_0,\xi_1}$ relative to $P^{(1)}_{\xi_0,\xi_1'}$ is easily calculated to be

$$\exp(-2|y_0y_1|)\exp[-2|y_1|W_2(t)/(1-t)].$$

Thus since $W_2(T)=\varepsilon^{-1/2}f(\varepsilon^{1/2}W_1(T))$, we have

$$(2.6)\qquad P^{(1)}_{\xi_0,\xi_1}\{T<1\}\exp(2|y_0y_1|) = E^{(1)}_{\xi_0,\xi_1'}\left\{\exp\left[\frac{-2|y_1|f(\varepsilon^{1/2}W_1(T))}{\varepsilon^{1/2}(1-T)}\right];\ T<1\right\}$$

(cf. Siegmund, 1985, Proposition 3.12).

Since

$$(2.7)\qquad \varepsilon^{-1/2}f(\varepsilon^{1/2}x)\sim\varepsilon^{1/2}f''(0)x^2/2\to 0\quad(\varepsilon\to 0),$$

for all sufficiently small $\varepsilon, P^{(1)}_{\xi_0,\xi_1'}\{T < 1\} = 1$, and the right hand side of (2.6) can be expanded to become

$$(2.8) \qquad 1 - |y_1|\varepsilon^{1/2} f''(0) E^{(1)}_{\xi_0,\xi_1'}[W_1^2(T)/(1-T)] + \dots .$$

Define

$$(2.9) \qquad \tau = \inf\{t : W_2(t) \geq 0\}.$$

From (2.7) follows $P^{(1)}_{\xi_0,\xi_1'}\{T_\varepsilon \to \tau\} = 1$, and hence (one expects that)

$$(2.10) \qquad E^{(1)}_{\xi_0,\xi_1'}[W_1^2(T)/(1-T)] \to E^{(1)}_{\xi_0,\xi_1'}[W_1^2(\tau)/(1-\tau)].$$

It is easy to see that conditional on $W_2(t), t \leq \tau, W_1(\tau)$ is distributed as $[\tau(1-\tau)]^{1/2} Z + x_0 + (x_1 - x_0)\tau$, where Z has a standard normal distribution. Hence

$$(2.11) \qquad \begin{aligned} E^{(1)}_{\xi_0,\xi_1'}[W_1^2(\tau)/(1-\tau)] &= x_0^2 + (1 + 2x_0x_1 - x_0^2) E^{(1)}_{\xi_0,\xi_1'}(\tau) \\ &\quad + x_1^2 E^{(1)}_{\xi_0,\xi_1'}[\tau^2/(1-\tau)]. \end{aligned}$$

Equation (2.5) follows from (2.6), (2.8), (2.10), (2.11), and the evaluations given below in Lemma 1.

To make the proceeding manipulations into a proof, one must consider the remainders in (2.7) and (2.8), and justify the convergence indicated in (2.10).

Let $A = \{\max_{t \leq T} |W_1(t)| \leq \varepsilon^{-1/4}\}$. From the distribution of the maximum of a pinned Brownian motion (e.g., Siegmund, 1985, (3.13)), it is easy to see that

$$(2.12) \qquad P^{(1)}_{\xi_0,\xi_1}(A^c) + P^{(1)}_{\xi_0,\xi_1'}(A^c) = o(\varepsilon^k) \quad \text{for all } k > 0.$$

Hence (2.6) can be replaced by

$$(2.13) \qquad \begin{aligned} &P^{(1)}_{\xi_0,\xi_1}\{T < 1\} \exp(-2|y_0 y_1|) \\ &\quad = E^{(1)}_{\xi_0,\xi_1'}\left\{\exp\left[\frac{-2|y_1| f(\varepsilon^{1/2} W_1(T))}{\varepsilon^{1/2}(1-T)}\right];\ \{T < 1\} \cap A\right\} + o(\varepsilon^k) \end{aligned}$$

for all $k > 0$. Let $\delta > 0$. By (2.12) and two applications of Taylor's theorem with remainder along the lines suggested in (2.7) and (2.8) one can obtain upper and lower bounds for the right hand side of (2.13) in the form

$$1 - |y_1|\varepsilon^{1/2}[f''(0) \pm \delta]E^{(1)}_{\xi_0,\xi'_1}[W_1^2(T)/(1-T);\ A] + o(\varepsilon^k).$$

Since $\delta > 0$ is arbitrary, by (2.11) and Lemma 1 below it suffices to show (cf. (2.10))

$$E^{(1)}_{\xi_0,\xi'_1}[W_1^2(T)/(1-T);\ A] \to E^{(1)}_{\xi_0,\xi'_1}[W_1^2(\tau)/(1-\tau)],$$

where τ is defined by (2.9). Since $P^{(1)}_{\xi_0,\xi'_1}\{T_\varepsilon \to \tau\} = 1$ and by (2.12) $P_{\xi_0,\xi'_1}(A) \to 1$, it suffices to show

$$\{1_A W_1^2(T)/(1-T);\quad \varepsilon > 0\} \tag{2.14}$$

is uniformly integrable.

Let $\tau' = \inf\{t : W_2(t) \geq |y_1|/2\}$. For all sufficiently small ε $A \subset \{T < \tau'\}$. It is easy to see that $[W_1(t) - x_0 - (x_1 - x_0)t]^2/(1-t)^2 - t/(1-t), 0 \leq t < 1$, is a martingale and hence $[W_1(t) - x_0 - (x_1 - x_0)t]^2/(1-t)^2, 0 \leq t < 1$, is a submartingale. From the joint distribution of τ' and $W_1(\tau')$ we obtain

$$E^{(1)}_{\xi_0,\xi'_1}\left\{[W_1(\tau') - x_0 - (x_1 - x_0)\tau']^2/(1-\tau')^2\right\} = E^{(1)}_{\xi_0,\xi'_1}[\tau'/(1-\tau')],$$

which is finite by Lemma 1 below. Also

$$E^{(1)}_{\xi_0,\xi'_1}\left\{[W_1(t) - x_0 - (x_1 - x_0)t]^2/(1-t)^2;\ \tau' > t\right\} = t(1-t)^{-1}P^{(1)}_{\xi_0,\xi'_1}\{\tau' > t\} \to 0$$

as $t \to 1$, again by Lemma 1. It follows from Doob's optional sampling theorem that on $\{T < \tau'\}$

$$\begin{aligned}&[W_1(T) - x_0 - (x_1 - x_0)T]^2/(1-T)^2 \\ &\qquad \leq E^{(1)}_{\xi_0,\xi'_1}\left\{[W_1(\tau') - x_0 - (x_1 - x_0)\tau']^2/(1-\tau')^2 \middle| W(t), t \leq T\right\}.\end{aligned}$$

Hence $\{1_{\{T<\tau'\}}[W_1(T) - x_0 - (x_1 - x_0)T]^2/(1-T)^2, \varepsilon > 0\}$ is uniformly integrable. The uniform integrability of (2.14) follows from the relation $A \subset \{T < \tau'\}$, the inequality $(a+b)^2 \leq 2(a^2 + b^2)$, and Lemma 1.

Lemma 1 provides justification for several steps in the preceding argument and evaluates the expectations appearing on the right hand side of (2.11). It will be convenient to use the following notation. Let $W(t), 0 \le t < \infty$, denote one dimensional Brownian motion with drift μ and initial value $W(0) = 0$. We write P_μ and E_μ to denote dependence of probabilities and expectations on μ. For $b > 0$ let $\tau_b = \inf\{t : W(t) \ge b\}$, where it is understood that $\inf\ \phi = +\infty$. Let $P_\xi^{(1)}(\cdot) = P_0(\cdot | W(1) = \xi)$.

Lemma 1. For $0 < t < 1$ the $P_\xi^{(1)}$ density function of τ_b is given by

$$f(t) = \frac{b}{[t^3(1-t)]^{1/2}} \varphi \left\{ b\left(\frac{1-t}{t}\right)^{1/2} - (\xi - b)\left(\frac{t}{1-t}\right)^{1/2} \right\} \tag{2.15}$$

For $\xi > b$

$$E_\xi^{(1)}(\tau_b) = b\Phi(-\xi)/\varphi(\xi)$$

and

$$E_\xi^{(1)}[\tau_b^2/(1-\tau_b)] = b/(\xi - b) - b\Phi(-\xi)/\varphi(\xi).$$

Proof. From the well known (and easily proved) fact that the $P_\xi^{(1)}$ distribution of $W(\cdot)$ is the same as the P_ξ distribution of $(1-(\cdot))W(\frac{(\cdot)}{1-(\cdot)})$, one easily sees that

$$\begin{aligned} P_\xi^{(1)}\{\tau_b \le t\} &= P_\xi\{(1-s)W[s/(1-s)] \ge b \quad \text{for some} \quad s \le t\} \\ &= P_{\xi-b}\{\tau_b \le t/(1-t)\}. \end{aligned}$$

Equation (2.15) follows by differentiation of the well known expression for the last probability (e.g., Siegmund, 1985, (3.15)).

From (2.15) one obtains

$$E_\xi^{(1)}[\tau_b^2/(1-\tau_b)] = b\int_0^\infty s^{-3/2}(1+s)^{-1}\varphi[(\xi-b)/s^{1/2} - bs^{1/2}]ds.$$

Writing $(1+s)^{-1} = \int_0^\infty e^{-\alpha(1+s)}d\alpha$, interchanging the order of integration, and using the well known equality

$$\int_0^\infty e^{-\alpha s} a s^{-3/2}\varphi(as^{-1/2} - \mu s^{1/2})ds = \exp\{-a[(2\alpha + \mu^2)^{1/2} - \mu]\}$$

(e.g., Siegmund, 1985, (3.16) and Problem 3.1), one obtains the given expression for $E_\xi^{(1)}[\tau_b^2/(1-\tau_b)]$. A similar calculation applies to $E_\xi^{(1)}(\tau_b)$.

Remarks. (i) As observed above, the boundary of $\mathcal{R}$ can be defined locally near $(0,0)$ by a function $y = f(x)$, but in general it cannot be so defined globally. However, for ε sufficiently small, on $\left\{\max_{0\le t\le\varepsilon}|W_1(t)| < \varepsilon^{1/4}\right\}$ T defined by (2.1) and the exit time from $\mathcal{R}$ coincide, so there is no loss of generality restricting attention to stopping times of this form. (ii) In higher dimensions, f'' in (2.4) becomes the Laplacian Δf, and $x_i^2 (i = 0,1)$ and $(x_1-x_0)^2$ become Euclidean distances $\| x_i \|^2$ $(i = 0,1)$ and $\| x_1 - x_0 \|^2$. The proof is essentially unchanged.

In Theorem 1 ξ_0 and ξ_1 are at a distance $O(\varepsilon^{1/2})$ from the boundary of $\mathcal{R}$ and from each other, and consequently $P_{\xi_0,\xi_1}^{(\varepsilon)}\{T<\varepsilon\}$ converges to a limit between 0 and 1. Theorem 2 is concerned with the case that ξ_0 and ξ_1 are fixed as $\varepsilon \to 0$, so $P_{\xi_0,\xi_1}^{(\varepsilon)}\{T<\varepsilon\} \to 0$.

As above, for given $\xi_0, \xi_1 \in \mathcal{R}$ suppose there exists a unique point on $\mathcal{R}$, the sum of whose distances from ξ_0 and ξ_1 is a minimum, and consider the tangent–normal coordinate system through this point. Let ξ_i have coordinates (x_i, y_i) $(i = 0,1)$, and let $\partial\mathcal{R}$ be given by the graph of $(x, f(x))$ in some neighborhood of $(0,0)$, so $f(0) = f'(0) = 0$.

Theorem 2. Assume f is twice continuously differentiable, $y_0y_1 > 0$, and

$$2y_0y_1f''(0)[1+(x_1/y_1)^2]/|y_0+y_1| > -1. \tag{2.16}$$

Let $T = \inf\{t : W(t) \in \partial\mathcal{R}\}$. Then as $\varepsilon \to 0$

$$P_{\xi_0,\xi_1}^{(\varepsilon)}\{T<\varepsilon\} \sim \frac{\exp(-2\varepsilon^{-1}y_0y_1)}{\{1+2y_0y_1f''(0)[1+(x_1/y_1)^2]/|y_0+y_1|\}^{1/2}}. \tag{2.17}$$

One can prove Theorem 2 along the lines of the proof of Theorem 1, but the details are rather different. To keep this paper to a reasonable length the proof has been omitted. An example comparing the numerical accuracy of (2.17) and (2.4) is given in Section 4.

An interesting case which fails to satisfy the conditions of Theorem 2 is $\mathcal{R}$ a disk with $\xi_0 = \xi_1$ at the center. In this case, the nearest point on $\partial\mathcal{R}$ is not unique and (2.16) is not satisfied. For an approximation in this case, which leans heavily on rotational symmetry,

see Siegmund (1985, Problem 11.1). An exact expression has been obtained by Kiefer (1959), but it is quite complicated.

A related but somewhat more complicated problem than that discussed in Theorem 1 is to approximate the joint distribution of $(T, W_1(T))$, which can be attacked via the characteristic function

$$E^{(\varepsilon)}_{\xi_0,\xi_1}[\exp\{i\lambda_1 W_1(T)/\varepsilon^{1/2} + i\lambda_2 T/\varepsilon\}; T < \varepsilon]. \tag{2.18}$$

Expansion of (2.18) to the precision of Theorem 1 seems to require more complicated calculations, which turn out to be very similar to those given in the following section in order to obtain the term of order ε in the expansion of $P^{(\varepsilon)}_{\xi_0,\xi_1}\{T < \varepsilon\}$.

It seems possible to obtain the results of this section by the methods of Jennen and Lerche (1981, 1982), but the computations appear to be somewhat more complicated. If one is interested in the joint behavior of T and $W_1(T)$, their method might turn out to be the simpler one.

3. The term of Order ε and Applications.

Calculation of higher order terms in the expansion (2.4) rapidly becomes very complicated in detail. In this section we see what is involved by examining the term of order ε. (See equation (3.10).) To simplify the algebra we suppose that $\xi_0 = \xi_1$. This special case sufficies for applications to the problems of Kac (1966) and Handelsman and Keller (1967), which are discussed below (cf. (3.15)). We proceed informally as in the first part of the proof of Theorem 1. The localization and uniform integrability arguments necessary for a rigorous proof are similar to those in Theorem 1 and have been omitted.

Let $\xi_0 = \xi_1$. In the notation of Section 2 for the standardized problem on the time interval $[0,1]$, (2.6) becomes

$$P^{(1)}_{\xi_0,\xi_0}\{T < 1\}\exp(2y_0^2) = E^{(1)}_{\xi_0,\xi_0'}\left\{\exp\left[\frac{-2|y_0|f(\varepsilon^{1/2}W_1(T))}{\varepsilon^{1/2}(1-T)}\right]\right\}, \tag{3.1}$$

where $\xi_0 = (0, y_0), \xi_0' = (0, |y_0|)$, and $T = T_\varepsilon$ is defined by (2.3). Assuming that f is three times continuously differentiable, we have

$$\varepsilon^{-1/2}f(\varepsilon^{1/2}x) = \varepsilon^{1/2}f''(0)x^2/2 + \varepsilon f'''(0)x^3/6 + o(\varepsilon);$$

and hence the right hand side of (3.1) becomes

$$(3.2)\quad 1-\varepsilon^{1/2}|y_0|f''(0)E^{(1)}_{\xi_0,\xi_0'}[W_1^2(T)/(1-T)]$$
$$-\frac{1}{3}\varepsilon|y_0|f'''(0)E^{(1)}_{\xi_0,\xi_0'}[W_1^3(T)/(1-T)]+\frac{1}{2}\varepsilon y_0^2[f''(0)]^2E^{(1)}_{\xi_0,\xi_0'}[W_1^4(T)/(1-T)^2]$$
$$+o(\varepsilon).$$

Until further notice, we shall write P and E for $P^{(1)}_{\xi_0,\xi_0'}$ and $E^{(1)}_{\xi_0,\xi_0'}$. Recall the definition of τ given in (2.9) and note that the conditional distribution of $W_1(\tau)$ given τ is normal with mean 0 and variance $\tau(1-\tau)$. Since $P\{T_\varepsilon\to\tau\}=1$ $(\varepsilon\to 0)$, we have

$$(3.3)\qquad E[W_1^3(T)/(1-T)]\to 0$$

and

$$(3.4)\qquad E[W_1^4(T)/(1-T)^2]\to 3E\tau^2.$$

Also

$$(3.5)\qquad E[W_1^2(T)/(1-T)]=E\tau+\{E[W_1^2(T)/(1-T)]-E[W_1^2(\tau)/(1-\tau)]\};$$

and the final contribution to the term of order ε in (3.2) comes from the difference on the right hand side of (3.5), which is itself of order $\varepsilon^{1/2}$.

First suppose that $f''(0)<0$ and to simplify some details that $f(x)\le 0$ for all x. The case $f''(0)>0$ involves a similar argument with slightly more complicated calculations. Let $\mathcal{F}_t$ denote the σ–algebra generated by $W(s), s\le t$. Since $T\le\tau$, we have

$$(3.6)\qquad E[W_1^2(\tau)/(1-\tau)]=E[(W_1(T)+W_1(\tau)-W_1(T))^2/(1-\tau)]$$
$$=E\left\{\frac{W_1^2(T)}{1-\tau}+\frac{2W_1(T)}{1-\tau}E[W_1(\tau)-W_1(T)|\mathcal{F}_T,\tau]+(1-\tau)^{-1}E[(W_1(\tau)-W_1(T))^2|\mathcal{F}_T,\tau]\right\}$$

Conditional on $\mathcal{F}_T$ and $\tau, W_1(\tau)-W_1(T)$ is normally distributed with mean $-W_1(T)(\tau-T)/(1-T)$ and variance $(\tau-T)(1-\tau)/(1-T)$. Hence after some algebra one obtains

$$(3.7)\qquad E[W_1^2(T)/(1-T)]-E[W_1^2(\tau)/(1-\tau)]$$
$$=E[(1-T)^{-2}W_1^2(T)E(\tau-T|\mathcal{F}_T)]-E[(1-T)^{-1}E(\tau-T|\mathcal{F}_T)].$$

Doob's optional sampling theorem yields

$$E\{(1-\tau)^{-1}[W_2(\tau)-W_2(T)-(\tau-T)(|y_0|-W_2(T))/(1-T)]|\mathcal{F}_T\}=0$$

(cf. Siegmund, 1985, Problem 3.12), and hence with probability one as $\varepsilon \to 0$

$$(3.8)\qquad E(\tau-T|\mathcal{F}_T)\sim \frac{\frac{1}{2}\varepsilon^{1/2}|f''(0)|W_1^2(T)(1-T)}{|y_0|+\frac{1}{2}\varepsilon^{1/2}|f''(0)|W_1^2(T)}$$
$$\sim \frac{1}{2}\varepsilon^{1/2}|y_0|^{-1}|f''(0)|W_1^2(\tau)(1-\tau).$$

Substitution of (3.8) into (3.7) yields

$$(3.9)\qquad E[W_1^2(T)/(1-T)]-E[W_1^2(\tau)/(1-\tau)]$$
$$\sim \frac{1}{2}\varepsilon^{1/2}|y_0|^{-1}|f''(0)|\{E[W_1^4(\tau)/(1-\tau)]-EW_1^2(\tau)\}$$
$$=\frac{1}{2}\varepsilon^{1/2}|y_0|^{-1}|f''(0)|\{3E[\tau^2(1-\tau)]-E[\tau(1-\tau)]\}.$$

From (3.1)-(3.5) and (3.9) we finally obtain

$$(3.10)\qquad P^{(1)}_{\xi_0,\xi_0}\{T<1\}=\exp(-2y_0^2)\Big\{1-\varepsilon^{1/2}|y_0|f''(0)E^{(1)}_{\xi_0,\xi_0'}(\tau)$$
$$+\frac{1}{2}\varepsilon[f''(0)]^2E^{(1)}_{\xi_0,\xi_0'}[3\tau^2(1-\tau)-\tau(1-\tau)+3y_0^2\tau^2]+o(\varepsilon)\Big\},$$

where T is defined by (2.3), τ by (2.9) $\xi_0=(0,y_0)$, and $\xi_0'=(0,|y_0|)$.

The expansion (3.10) also holds when $f''(0)>0$. In this case $\tau\le T$, so (3.6) must be replaced by

$$E[W_1^2(T)/(1-T)]=E[W_1^2(\tau)/(1-T)]$$
$$+2E\left\{W_1(\tau)E\left[\frac{W_1(T)-W_1(\tau)}{1-T}|\mathcal{F}_\tau\right]\right\}+E\left\{E\left[\frac{(W_1(T)-W_1(\tau))^2}{1-T}|\mathcal{F}_\tau\right]\right\}.$$

By optional sampling

$$E\left[\frac{W_1(T)-W_1(\tau)}{1-T}|\mathcal{F}_T\right]=-(1-\tau)^{-1}W_1(\tau)E[(T-\tau)/(1-T)|\mathcal{F}_\tau],$$

and it may be shown that

$$E\{[W_1(T) - W_1(\tau)]^2/(1-T)|\mathcal{F}_\tau\} \sim E[(T-\tau)/(1-T)|\mathcal{F}_\tau].$$

Hence in place of the equality (3.7) one obtains

$$\begin{aligned} &E[W_1^2(\tau)/(1-\tau)] - E[W_1^2(T)/(1-T)] \\ &\sim E[(1-\tau)^{-2}W_1^2(\tau)E(T-\tau|\mathcal{F}_\tau)] - E[(1-\tau)^{-1}E(T-\tau|\mathcal{F}_\tau)]. \end{aligned}$$

A result similar to (3.8) holds for $E(T-\tau|\mathcal{F}_\tau)$, and the rest follows as before.

Remarks. (i) By the method of Lemma 1 one can evaluate the moments appearing on the right hand side of (3.1). However, for the applications given below, which in effect involve an integration of (3.10) over ξ_0, the computations are considerably simpler if one interchanges the order of the two integrations and integrates over ξ_0 first. (ii) In higher dimensions the relation of $\partial\mathcal{R}$ to its tangent planes can be more complicated than in two dimensions. In general, one must condition on $\mathcal{F}_{T\wedge\tau}$ and consider the two cases $\{T \le \tau\}$ and $\{T > \tau\}$. Whereas the term of order $\varepsilon^{1/2}$ involves only the Laplacian of f, i.e., the mean curvature of $\partial\mathcal{R}$, the term of order ε involves mixed partials as well. For the problem studied by Handelsman and Keller (1966), where $\mathcal{R}$ is the region exterior to a sphere in $\mathbb{R}^3$ one does not encounter these complications.

Now let T denote the first exit time of W from $\mathcal{R}$, and for $\xi_0, \xi_1 \in \mathcal{R}$ define $p(t, \xi_0, \xi_1)$ by

$$p(t,\xi_0,\xi_1)d\xi_1 = \Pr(T > t, W(t) \in d\xi_1 | W(0) = \xi_0).$$

Observe that

$$p(t,\xi_0,\xi_0) = (2\pi t)^{-d/2}[1 - P^{(t)}_{\xi_0,\xi_0}\{T < t\}]. \tag{3.11}$$

In order to study (1.2) in a bounded region $\mathcal{R}$ in $\mathbb{R}^2$ Kac (1966) uses the representation

$$\sum \exp(-\lambda_k t) = \iint_{\mathcal{R}} p(t,\xi_0,\xi_0)d\xi_0,$$

which by (3.11) equals

$$(2\pi t)^{-1}[|\mathcal{R}| - \iint_{\mathcal{R}} P^{(t)}_{\xi_0,\xi_0}\{T < t\}d\xi_0], \tag{3.12}$$

where $|\mathcal{R}|$ denots the area of $\mathcal{R}$. Handelsman and Keller (1966) are interested in $I\!R^3$ and the integral

$$\iiint_{\mathcal{R}} [1-(2\pi t)^{3/2} p(t,\xi_0,\xi_0)] d\xi_0,$$

which by (3.11) equals

$$\iiint_{\mathcal{R}} P^{(t)}_{\xi_0,\xi_0}\{T<t\} d\xi_0. \tag{3.13}$$

In order to analyze the integral in (3.12) it is convenient to make a change of variables (cf., Pleijel, 1954) to obtain

$$\iint_{\mathcal{R}} P^{(t)}_{\xi_0,\xi_0}\{T<t\} d\xi_0 = \int_{\partial\mathcal{R}} \int_0^{\delta} P^{(t)}_{\xi_0,\xi_0}\{T<t\}[1-|y_0|c(\sigma)] d|y_0| d\sigma + 0(e^{-2\delta^2/t}), \tag{3.14}$$

where σ denotes arc length on $\partial\mathcal{R}, c(\cdot)$ is the curvature of $\partial\mathcal{R}$, and ξ_0 has coordinates $(0,y_0)$ in the tangent–normal coordinate system with its origin at the point σ of $\partial\mathcal{R}$, so $|y_0|$ is the distance from ξ_0 to $\partial\mathcal{R}$ and $c(\sigma)=-f''(0)$.

Keeping (2.2) and (2.15) in mind, one can substitute (3.10) into (3.14), integrate with respect to $|y_0|$, then with respect to σ, and refer to the Gauss–Bonnet theorem as indicated by Kac to obtain

$$\begin{aligned}\sum \exp(-\lambda_k t) &= (2\pi t)^{-1}|\mathcal{R}| - [4(2\pi t)^{1/2}]^{-1}|\partial\mathcal{R}| \\ &\quad + (1-h)/6 + 2^{-8}(2\pi)^{-1/2}\left(\int_{\partial\mathcal{R}} c^2(\sigma)d\sigma\right)t^{1/2} + o(t^{1/2}),\end{aligned} \tag{3.15}$$

where $|\partial\mathcal{R}|$ is the length of $\partial\mathcal{R}$ and h is the number of holes in $\mathcal{R}$.

Since (3.15) involves integration of (3.10), some additional justification is required to claim that (3.15) has been proved rigorously. This seems a straightforward, albeit rather technical matter. Since it does not appear to add significant insight, the details are omitted.

The expansion (3.15) agrees with those given by Stewartson and Waechter (1971) and Smith (1981), both of whom used analytical methods and obtained additional terms. The term of order $t^{1/2}$ disagrees with that given by Louchard (1968), whose argument appears to contain an improper use of the Markov property.

A similar computation yields the expansion of Handelsman and Keller (1966).

4. Monte Carlo Methods.

Again let $W(t)$ denote Brownian motion starting from some point inside a region $\mathcal{R}$ in d-dimensional Euclidean space, and let $T = \inf\{t : W(t) \notin \mathcal{R}\}$. In this section we consider the problem of estimating by Monte Carlo methods probabilities like

$$\Pr\{T \leq t\}. \tag{4.1}$$

The same ideas are applicable to substantially more complicated first passage distributions.

An obvious procedure to estimate (4.1) is to partition the time interval $[0, t]$ by the points $t_i = i\varepsilon$, $i = 0, 1, \ldots, m$, where $\varepsilon = t/m$, generate N realizations of the discrete time random walk $W(t_i)$, $i = 0, 1, \ldots, m$, and estimate (4.1) by the relative frequency among the N realizations that $W(t_i) \notin \mathcal{R}$ for some $1 \leq i \leq m$.

The standard deviation of this estimator is of order $N^{-1/2}$. Its bias equals the difference between $\Pr\{W(t_i) \notin \mathcal{R} \quad \text{for some} \quad 1 \leq i \leq m\}$ and (4.1), which presumably is of order $\varepsilon^{1/2}$ (cf. Nagaev, 1970, Siegmund, 1985, Chapter X, Hogan, 1984). Thus the bias is of the same order as the sampling error unless ε is small compared to N^{-1}. Since N may be in the thousands, it is often computationally unfeasible to achieve a satisfactory estimate by the obvious device of making ε extremely small.

The procedure we propose to study is the following. Having generated the partial realization $W(t_0), \ldots, W(t_i)$ and decided that $T > t_i$, generate $W(t_{i+1})$. If $W(t_{i+1}) \notin \mathcal{R}$ decide $T \leq t_{i+1} \leq t$. If $W(t_{i+1}) \in \mathcal{R}$ decide $T \leq t_{i+1} \leq t$ with probability $p[W(t_i), W(t_{i+1}), \varepsilon]$, where $p(\xi_0, \xi_1, \varepsilon)$ is a suitable approximation for $P^{(\varepsilon)}_{\xi_0,\xi_1}\{T < \varepsilon\}$ obtained from Theorem 1.

As a first example we consider a rather complicated, but linear problem. In this case there is no question how carefully one should approximate $P^{(\varepsilon)}_{\xi_0,\xi_1}\{T < \varepsilon\}$, which can be evaluated exactly; and we see that a striking improvement in the accuracy of the naive estimator is possible.

The example concerns

$$P^{(1)}_{0,\xi}\{\max_{0 \leq s < t \leq 1} [W(t) - W(s)] \geq b\}, \tag{4.2}$$

where W is one dimensional Brownian motion and b is substantially larger than $\max(0, \xi)$, so the probability (4.2) is small. This probability has arisen in the unrelated problems of

Levin and Kline (1985) and Adler and Brown (1986). Hogan and Siegmund (1986) show that if $b \to \infty$ and ξ varies with b in such a way that ξ/b is a fixed real number less than 1, then (4.2) equals

$$[2(2b-\xi)(b-\xi)+1+o(1)]\exp[-2b(b-\xi)]. \tag{4.3}$$

In order to check the accuracy of the approximation (4.3) by simulation, we first generate a $P_{0,\xi}^{(1)}$ realization of the discrete skeleton $W(i/m),\ i=0,1,\ldots,m$ and locate the points $0 \le \nu_1 < \nu_2 \le m$ which satisfy

$$W(\nu_2/m) - W(\nu_1/m) = \max_{0\le i<j\le m}[W(j/m)-W(i/m)].$$

Then for each $[(\nu_1+\nu_2)/2] \le i < m$ we generate the maximum of $W(t)$ for $i/m \le t \le (i+1)/m$, which conditional on $W(i/m)=\xi_0, W\{(i+1)/m\}=\xi_1$ has the distribution

$$P_{\xi_0,\xi_1}^{(m^{-1})}\{\max_{0\le t\le m^{-1}} W(t) \ge x\} = \exp[-2m(x-\xi_0)(x-\xi_1)]$$

for $x \ge \max(\xi_0,\xi_1)$. Similarly we generate minima over $[i/m,(i+1)/m],\ i=0,1,\ldots,[(\nu_1+\nu_2)/2]-1$. Putting $t^* = m^{-1}[(\mu_1+\nu_2)/2]$, we use

$$\max_{t^*\le t\le 1} W(t) - \min_{0\le t\le t^*} W(t) \tag{4.4}$$

as a surrogate for the desired

$$\max_{0\le s\le t}[W(t)-W(s)],$$

for which it is in fact a lower bound. Presumably the discrepancy between these two quantities is unimportant in the cases of primary interest, when (4.2) is small. As a check one might compare results for two different values of m, or alternatively perform a second experiment with the maxima and minima taken over overlapping sets of intervals, say $\nu_1 \le i < m$ and $0 \le i < \nu_2$, which in all but very few cases would yield an upper bound.

Table 1 gives the results of an experiment with $N = 9999$ repetitions. The first Monte Carlo estimate reported in each row is the relative frequency of the event $\{\max_{0\le i<j\le m}[W(j/m) - W(i/m)] \ge b\}$; the second is the modified estimate described above. The final entry in each row gives the approximation (4.3). There is wide disparity between the discrete

skeleton estimator and the modified estimator, and except for two cases there is excellent agreement between the latter estimator and the theoretical approximation. Those two discrepancies both involve large probabilities, where (4.3) is not expected to provide a good approximation.

For a second example we consider the first hitting time of a sphere of radius r by a three dimensional Brownian motion starting outside the sphere. This problem is surrogate for a much more elaborate problem in physical chemistry (N.J.B. Green, personal communication). In that problem n independent spheres of radius r' follow independent Brownian paths, annihilating each other if they collide. Our problem is the spescial case $n = 2$ and $r = 2r'$. Moreover, if one simulates a sequence of snapshots of the configurations of the n spheres at times $i\varepsilon$ $(i = 0, 1, \ldots, .)$, it seems plausible that one can bridge the short gap from $i\varepsilon$ to $(i+1)\varepsilon$ by considering each pair of spheres in isolation from the others, and hence the case $n = 2$ may be useful preparation for other cases.

In order to implement the proposed algorithm one must choose an approximation for

$$(4.5) \qquad P^{(\varepsilon)}_{\xi_0,\xi_1}\{\min_{0\leq t\leq \varepsilon} \| W(t) \| \leq r\}.$$

Since the approximation of Theorem 1 requires some numerical computation to determine the point on the surface of the sphere the sum of whose distances from ξ_0 and ξ_1 is a minimum, it seems reasonable to try first the simpler approximation which treats the surface of the sphere as a plane and approximates (4.5) by the very simple

$$(4.6) \qquad \exp[-2(\| \xi_0 \| - r)(\| \xi_1 \| - r)/\varepsilon].$$

Under the asymptotic scaling of Theorem 1, (4.6) and (2.4) have the same limits, but differ at the term of order $\varepsilon^{1/2}$.

As indicated above, there is reason to think that the bias of a direct frequency count from the discrete skeleton is of order $\varepsilon^{1/2}$ and hence requires one to take $\varepsilon \cong N^{-1}$, the number of repetitions of the experiment. Although we have no idea how to prove it, we believe that use of (4.6) to bridge the gaps in the discrete skeleton results in an estimator whose bias is of order ε, and use of the better approximation of Theorem 1 reduces this bias to order $\varepsilon^{3/2}$. If these conjectures are true, then even if the simple approximation

(4.6) is used, a reasonable magnitude for ε is about $N^{-1/2}$, which represents a considerable improvement.

Table 2 reports the results of a simulation experiment to estimate (4.1) for the hitting time T of a sphere of radius r by a three dimensional Brownian motion starting from the point $(x, 0, 0)$. The interval width of the discrete skeleton is ε. The Monte Carlo estimators are based on $N = 9999$ repetitions of the method described above with the simple approximation (4.6). The exact probabilities,

$$\Pr(T \leq t) = 2x^{-1}r\{1 - \Phi[(x-r)/t^{1/2}]\},$$

are also included. The approximations are quite accurate, in fact more accurate than one would expect from the conjectured size of the bias.

Our final example is designed to discover whether we can gain anything by using the presumably better approximation provded by Theorem 1 to bridge the gap between $W(t_i)$ and $W(t_{i+1})$. To simplify the programming problem of determining the local tangent-normal coordinate systems associated with the points $W(t_i) = \xi_0$ and $W(t_{i+1}) = \xi_1$, we take $d = 2$ and T the first time $W(t)$ is within a circle of radius r centered at the origin. In order to investigate at the same time the numerical accuracy of the approximations of Theorems 1 and 2, we study the conditional probabililty, $P^{(1)}_{\xi_0,\xi_0}\{T < 1\}$.

For $\mathcal{R}$ the region exterior to a circle of radius r, $f''(0) \equiv r^{-1}$. It seems plausible that one might improve the numerical accuracy of (2.4) slightly by including the term of order $\varepsilon^{1/2}$ in the exponent to obtain

$$(4.7) \qquad P^{(\varepsilon)}_{\xi_0,\xi_1}\{T < \varepsilon\} \cong \exp\Bigg\{ -2\varepsilon^{-1}|y_0 y_1| - r^{-1}\Bigg[\varepsilon^{-1/2}|y_0 y_1| \times \frac{\Phi[\varepsilon^{-1/2}(y_0+y_1)]}{\varphi[\varepsilon^{-1/2}(y_0+y_1)]}[(1-\varepsilon^{-1}(x_0-x_1)^2] + \varepsilon^{-1}(x_0^2|y_1| + x_1^2|y_0|)\Bigg]\Bigg\}.$$

Table 3 contains the results of an experiment with $r = 1$ and $N = 9999$ repetitions. There is no evidence that the more complicated approximation yields more accurate Monte Carlo estimates. Since the additional numerical computation required to evaluate (4.7) after each new observation more than doubles the total computational effort, there does

not seem to be any reason to use this approximation, at least for the relatively simple problem considered here.

As expected, the analytical approximation provided by Theorem 1 is better than that of Theorem 2 when $P^{(1)}_{\xi_0,\xi_0}\{T < 1\}$ is large or moderate, and the converse is true when this probability is small. Overall, the better of the two approximations is reasonably good.

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Table 1

Evaluation of $P^{(1)}_{0,\xi}\{\max_{0\le s<t\le 1}[W(t)-W(s)]\ge b\}$

b	ξ	m $(=\varepsilon^{-1})$	Monte Carlo Estimates: Discrete	Monte Carlo Estimates: Interpolated	Approximation (4.3)
.671	-1.79	20	.136	.501	.605
.894	-1.79	20	.029	.158	.166
1.118	-1.79	20	.006	.035	.037
.671	-1.79	80	.288	.544	.605
.894	-1.79	80	.071	.163	.166
1.118	-1.79	80	.013	.038	.037
1.095	0.0	30	.257	.520	.526
1.278	0.0	30	.114	.287	.287
1.461	0.0	30	.048	.127	.134
1.278	.548	30	.356	.610	.608
1.461	.548	30	.177	.372	.371
1.643	.548	30	.074	.195	.191

Table 2

First Passage to a Sphere

r	x	ε	t	$\Pr(T \le t)$		t'	$\Pr(T \le t')$	
				Monte Carlo	Exact		Monte Carlo	Exact
2	3	.50	1	.2110	.2115	9	.5016	.4926
2	3	.25	1	.2162	.2115	9	.4996	.4926
4	6	.50	2	.0986	.1049	25	.4495	.4594
4	7	.25	2	.1004	.1049	25	.4597	.4594

Table 3

Approximations for $P^{(1)}_{\xi_0,\xi_0}\{\min_{0\le t\le 1} \| W(t) \| \le 1\}$

$\| \xi_0 \|$	Monte Carlo Estimates				Analytic Approximations	
	Using (4.6)		Using (4.7)		(4.7)	(2.17)
	$\varepsilon = .1$	$\varepsilon = .05$	$\varepsilon = .1$	$\varepsilon = .05$		
1.2	.866	.891	.856	.889	.889	.843
1.5	.536	.535	.524	.538	.515	.495
2.0	.097	.106	.095	.102	.089	.096

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Let T be the first exit time of Brownian motion $W(t)$ from a region $\mathcal{R}$ in d-dimensional Euclidean space having a smooth boundary. Given points ξ_0 and ξ_1 in $\mathcal{R}$, ordinary and large deviation approximations are given for $\Pr\{T < \epsilon | W(0) = \xi_0, W(\epsilon) = \xi_1\}$ as $\epsilon \to 0$. Applications are given to hearing the shape of a drum, approximating the second virial coefficient, and Monte Carlo estimation of first passage distributions for Brownian motion.

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